Abstract No. cele711

**Structural Investigation of the Mineral Welshite**

A. Celestian (SUNY, Stony Brook), E. Grew (U. of Maine), J. Parise (SUNY, Stony Brook), and G. Wu (SUNY, Buffalo)

Beamline(s): X3A1

**Introduction:** The mineral Welshite is triclinic inosilicate of the Aenigmatite group with a composition of Ca2 Mg3.8 Mn0.6 Fe0.1 Sb1.5 O2 [Si2.8 Be1.7 Fe0.65 Al0.7 As0.17 O18] [1]. This rare mineral coming from Langban, Sweden, is suggested to have an abundance of Be in tetrahedral coordination, and antimony in the crystal. To locate the Be site and its coordination, single crystal diffraction at a synchrotron is needed.

**Methods and Materials:** A 20x30x20 micron crystal of Welshite, with the chemical composition above, was mounted on a small cactus needle with epoxy into a standard goniometer pin. The cactus needle was chosen for its sharp point, needed for mounting micro crystals, and for its low scattering power which does not contribute significant background to the diffraction pattern. Helium gas was used, and injected into the collimator, to reduce air scattering that contributes to large background counts. A Bruker 6K CCD detector was used to collect the data at a distance of 4.2 cm from the crystal. 1250 frames were collected around the phi axes with a .3 degree frame width at a wavelength of .394 angstroms. SAINT [2]was used to reduce the raw data from the area detector, SADABS [3] was used for absorption corrections, SHELXTL [4] was used for structure solution and GEMINI suite of programs was used to check for twinning. Data was collected at room temperature.

**Results:** After data collection, a unit cell was found to be triclinic a=8.9747 b=9.9048 c=10.5078 alpha=64.169 beta=86.218 and gamma=64.818 (cell lengths in angstroms and angles in degrees). After solving the structure, it was clear that the crystal was either twinned or cracked. Using GEMINI, we found that the crystal was cracked at ..15 degrees apart. After assigning the diffracted spots to each crystal half, the structure was still unclear. This may be due to the iron/beryllium disorder in the tetrahedral site.

**Conclusions:** Due to the chemical and structure complexity, the structure of welshite has not been solved. Further analyses into possible twinning types and order/disorder relationships are underway

**Acknowledgements:** This work was supported through a grant from the National Science Foundation #DMR-0095633. Also thanks SUNY X3 beamline at NSLS is supported by the Division of Basic Energy Sciences of the US Department of Energy (DE-FG02-6ER45231).

**Reference:**

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